HRTEM, Z-CONTRAST AND ATOMISTIC MODELLING: A QUANTITATIVE STUDY ON THE Σ5 (310)/[001] STGB IN CU DOPED AL

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To determine the atomistic structure at the Σ5 (310)/[001] symmetric tilt grain boundary (STGB) in copper doped (1at%) aluminum we used HRTEM in combination with focal-series reconstruction (FSR), Z-contrast imaging and theoretical ab-initio calculations.
Nowadays, field emission microscopes are widely spread and very popular because of their advantages over thermionic emitters (high brightness, very coherent electron beam, etc.). However, the interpretation of HRTEM images obtained with field emission sources is not straightforward because the image is a highly encoded mixture out of TEM and object properties. To overcome this, we can use FSR of the exit wave function to exclude the imaging artifacts[1,2]. Additionally, FSR can provide not only detailed information on the atomic structure but also chemical information related to the projected potential (Z = atomic number) of the elements under investigation[3].
On the other hand, Z-contrast imaging is another comparable method, which combines the information of the atomic structure and the chemistry. However, the image formation mechanisms of Z-contrast imaging or incoherent imaging and HRTEM are completely different in their nature and both techniques hold likewise advantages and disadvantages. Thus, one major goal in our study is to reveal and demonstrate the enormous possibilities implied by the combination of these two complementary experimental techniques in material science. In addition we focus in the comparison with theoretical calculations particularly to validate the predictions of the theoretical grain boundary model.
For our study we have chosen a model grain boundary fabricated with ultra-high vacuum diffusion bonding[4] of single crystals to investigate the segregation of an impurity (Cu) to distinct sites in a special Al grain boundary (Σ5 (310)/[001] STGB). Segregation is of long standing scientific interest and it is known that segregation can

alter material properties in dramatic ways. For instance, one of the major controlling factors for electromigration (EM) is expected to be the segregation of Cu atoms to Al grain boundaries (GB) [5,6].

Investigations were performed using mainly the Philips CM 300 FEG ST at LLNL and the Philips CM 300 FEG UT at the NCEM, both equipped with an Gatan Imaging Filter (GIF). Additionally, we have performed Z-contrast investigations using the dedicated STEM VG HB603 U operated at 300kV, equipped with a cold field emitter and a high resolution objective lens operated at the Oak Ridge National Laboratory (ORNL). The atomic structures were modeled with atomistic potentials based on the Embedded Atom Method (EAM), where we used a mixed basis set within the Local Density Approximation (LDA).

The reconstruction of the Al-1at%Cu grain boundary revealed a structure, which was previously not considered. However, the possibility of an interstitial has been mentioned in literature[7,8], but our experimental results validate for the first time the predicted model. We will present and compare our experimental findings with the modeled systems in detail and we will discuss our observations with respect to earlier presented results[9,10].

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